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New information from bremsstrahlung: new calculations for new experiments

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Abstract: We review approaches to the description of bremsstrahlung and the extent to which they are in accord with present experimental information. Beyond simple Born approximation predictions, the standard theoretical approach for the doubly differential cross section at x-ray and soft γ-ray energies is based on the relativistic independent-particle-approximation code of Tseng. There are new results at low energies, both where a classical domain is approached and at energies comparable to transition energies, where the correlation effects of polarizational bremsstrahlung can dominate. Recently Tseng's code has been extended, by rearranging the manner in which radial matrix elements are summed, to provide predictions for the triply differential cross section, viewed as providing a more sensistive probe of the validity of external-field quantum electrodynamics. We discuss the types of information we are learning about the atom and about classical, nonrelativistic and relativistic quantum descriptions of these processes.

Keywords: bremsstrahlung, x-ray radiation, gamma-ray radiation

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1. Introduction

We describe here some of the newer issues in the description of the bremsstrahlung process. In Sec. 2 we give a simplified description of the variables which characterize this process. In Sec. 3 we describe the earlier theoretical approaches to the description of bremsstrahlung which still prove useful. In Sec. 4 we describe the relativistic independent-particle-approximation (IPA) calculations which currently form the basis of our most complete description of the bremsstrahlung spectrum and doubly differential cross section, through the x-ray and soft γ-ray regimes. We then describe newer work. In Sec. 5 we discuss the situation at lower energies, whether described classically or in terms of a few multipole matrix elements, and then the circumstances of polarizational bremsstrahlung, causing modifications due to the response of the atomic target. In Sec. 6 we describe the recent extension of the IPA calculations to the triply differential cross section, expected to be more sensitive to the nature of the basic external-field-quantum-electrodynamic (QED) interaction. Finally, In Sec. 7 we discuss what can be learned from studies of bremsstrahlung, both in terms of how much bremsstrahlung tells us about atomic structure and its responses, and in terms of the extent to which classical, nonrelativistic and relativistic formulations matter.

2. The process and its observables

We are restricting our considerations to circumstances in which a low-density electron beam is incident on well separated atoms or ions, so that we may describe the situation in terms of a single electron incident on a single target atom. Then if we make the further approximation of describing the target atom as unchanging, described solely in terms of an atomic potential in which the incident electron scatters, conservation of energy will be described as the transfer of energy from the incident electron to the scattered electron and radiated photon. In principle we should distinguish between an inclusive reaction, in which atomic changes are not observed, and an exclusive reaction, in which the atomic state is established to be unaltered. A simple description, as replacing the atom by a potential, can generally be understood as an inclusive description. When we give a more definite description of the atomic state, as in polarizational bremsstrahlung, we will need to specify explicitly whether we have an inclusive or an exclusive process in mind.

At this level the process is specified by the target (its charge, whether neutral or ionic), the initial and final electron momentum and spin $(\boldsymbol{p}_i, s_i)$ and $(\boldsymbol{p}_f, s_f)$ and the photon momentum and polarization $(\boldsymbol{k}, \bar{\varepsilon})$. If we assume an unpolarized incident beam and no detection of spin and polarization in the final state, then the observables are:

triply differential cross section

$$d^3\sigma \equiv \frac{d^3\sigma}{dk\,d\Omega_k\,d\Omega_f}$$

doubly differential cross section for bremsstrahlung

$$d^2\sigma \equiv \frac{d^2\sigma}{dk\,d\Omega_k} \equiv \int \frac{d^3\sigma}{dk\,d\Omega_k\,d\Omega_f}\,d\Omega_f$$

bremsstrahlung energy spectrum

$$d\sigma \equiv \frac{d\sigma}{dk} \equiv \int \frac{d^2\sigma}{dk\,d\Omega_k}\,d\Omega_k$$

or, spectrum of energy intensity radiated

$$\sigma \equiv \left(\frac{\beta_i^2 k}{Z^2}\right)\frac{d\sigma}{dk}$$

or, Gaunt factor

$$g \equiv \frac{\sigma}{5.61\,\mathrm{mb}}$$

energy loss

$$\mathrm{E.L.} \equiv \frac{1}{E}\int_0^{T_i} k\,\frac{d\sigma}{dk}\,dk$$

3. Earlier stages in the development of predictions

We will briefly mention some of the earlier theoretical work on bremsstrahlung which remains useful in our current understanding of the process. For more details some of the standard review articles should be consulted [1].

Classical predictions for the spectrum in a Coulomb potential were given (in a footnote) by Kramers [2]; the derivation is given in some detail by Landau and Lifshitz [3]. The soft-photon limit is the universal logarithm, the hard-photon limit the (constant) Kramers formula. The angular distribution in this Coulomb case has been discussed more recently [4]. Classical predictions for the spectrum and angular distribution in screened potentials are discussed in Sec. 5.

Nonrelativistic quantum mechanics for the Coulomb potential leads to the Sommerfeld formula for the spectrum [5], assuming dipole approximation; the corresponding angular distribution has been tabulated. For small $Z\alpha/\beta$ the Sommerfeld formula reduces to nonrelativistic Born approximation, and from the two the Elwert factor [6] was derived as a simple correction to the Born approximation. Numerical codes have been written to perform the calculation in screened potentials [7], but they do not appear to have been widely used. We note the more recent nonrelativistic code of Tseng for $d^3\sigma$ [8]. In Born approximation the result in a screened potential is obtained from the Coulomb Born result by multiplying by the square of the form factor. Usually the Elwert factor is also applied.

Relativistic quantum mechanics for the Coulomb potential in Born approximation leads to the Bethe-Heitler formula, available for σ, $d^2\sigma$ and $d^3\sigma$ [9]. Usually the Elwert factor is applied. The high energy limit in the Coulomb potential was obtained, using Sommerfeld-Maue wave functions, by Bethe and Maximon [10]. Result of this type were generalized by Elwert and Haug [11], obtaining an interpolating form valid both for all Z at high energies and for small Z at all energies, usable to some extent at intermediate energies, available for σ, $d^2\sigma$ and $d^3\sigma$. Usually a form factor is applied to account for screening. Relativistic numerical calculations in screened potentials are described in the next section.

The hard and soft radiated photon situations (most or little of the incident electron energy radiated) are related to other atomic processes, which provide additional information regarding bremsstrahlung. When little energy is radiated, the bremsstrahlung matrix element is related through the low-energy theorem to the matrix element for elastic electron scattering [12]. When most of the energy is radiated, the matrix element is an analytic continuation of that for direct radiative recombination, and so also to its inverse, atomic photoeffect [13].

4. Relativistic IPA calculations for the doubly differential cross section

As we wrote in 1985 [1], and as is still true, "the best available results for σ and $d^2\sigma$, for incident energies 500 eV to 10 MeV and all elements, have been obtained from a relativistic numerical calculation of the matrix element M in partial waves and multipoles, treating the process in a Dirac-Slater central potential, with local Kohn-Sham exchange and no Latter tail in the neutral atom case. The code was developed by Tseng [14], who also obtained most of the base data which have subsequently made tabulation of predictions possible [15]." Further results for ions have been obtained with the code [16]; and extension and reformulation of the code to calculate $d^3\sigma$ is described in Sec. 6.

5. Recent work at low energies

Classical predictions for the spectrum and angular distribution in bremsstrahlung have been obtained in screened potentials [17]. The same assumptions were made as in the Coulomb case (i.e. trajectories calculated in the potential as a function of impact parameter), neglecting energy loss, obtaining the spectrum as the Fourier transform of the radiation distribution, integrated over impact parameters). Just as in the Coulomb case, the validity of classical screened results for the spectrum persists into the x-ray regime (10 keV). This permits simple parameterizations [18]. Classical semi-analytical approaches have also been developed, based on the so-called Kramers electrodynamics, which offer the possibility of insight into the underlying mechanisms in these regimes. In the numerical calculations it was also observed [17] that the angular distribution begins to oscillate rapidly as a function of energy for electron energies of a few eV. In more recent work, Shaffer [19] has shown that similar oscillations are occurring in the intensity of the spectrum and that both phenomena are related to the energy at which classical resonance (trapping) can occur. In the corresponding quantum case, shape resonances have been seen for suitable potentials [20], when the outgoing electron is of suitably low energy. They are only exposed when the incoming electron energy is low enough that suitable angular momenta (not just s states) contribute in the outgoing state.

Another phenomena in low-energy quantum matrix elements are zeroes, leading to minima in cross sections. These Cooper minima are well known in photoeffect, but they also occur in bremstrahlung and inverse bremstrahlung. An eveness oddness argument for the number of such zeroes can be given for bremsstrahlung, along similar lines to the argument earlier given for photoeffect [21]. Since soft photon bremsstrahlung is related to elastic scattering through the low energy theorem, there are corresponding zeroes in the elastic-scattering matrix elements. Observability of such zeroes requires that it is a dominant matrix element which has a zero. Examples have been given in bremsstrahlung; a corresponding case in elastic scattering is a Ramsauer-Townsend minima.

In the low-energy regimes one can also expect phenomena involving radiation from the structure of the atom, i.e. via many-body correlations, now generally called polarizational bremsstrahlung [22], as contrast to radiation off the projectile accelerating in the atomic potential.. The simplest situation can be described in terms of a virtual photon scattering off the atomic electrons. Available experimental confirmation of this phenomenon is limited, but new experiments are anticipated. We note, by contrast, that in ion-atom collisions, potential bremsstrahlung is reduced by the mass of the ion; polarizational bremsstrahlung is not and has clearly been seen.

6. Recent work on the triply differential cross section

Recently the relativistic bremsstrahlung code of Tseng and Pratt was extended and reformulated to permit a calculation of the triply differential bremsstrahlung cross section $d^3\sigma$, corresponding to electron-photon coincidence measurements in electron scattering on neutral atoms [23]. The extension involved a different organization of the partial-wave and multipole summations, performing the summations on the matrix element rather than the cross section. This exploits the knowledge that the cross section is a perfect square (of the matrix element), cutting the number of summations in half, at the price of performing summations or integrations over quantities not observed numerically rather than analytically. The prior approach is much better for $d^2\sigma$, the latter approach much better for $d^3\sigma$.

It is often argued [1] that $d^3\sigma$ provides a more stringent test of the underlying theory from description of the interaction than $d^2\sigma$, since in summation sensitivity to the details of the interaction can be lost. The limited available information on $d^3\sigma$, corresponding to coincidence measurements of electron scattering through an angle θ_e, with a photon radiated in the plane at angle θ_γ, has been summarized by Shaffer et al. [23] and compared with the new theoretical predictions and the previously available Elwert-Haug results [11]. There is no systematic agreement agreement among these results, particularly for $Z = 79$ but also for $Z = 47$.

We illustrate these situations in Figs. 1-3. In Figs. 1-2 examples of cross sections in coplanar geometry are shown, according to the calculations of Shaffer et al., the predictions of the theory of Elwert and Haug with form

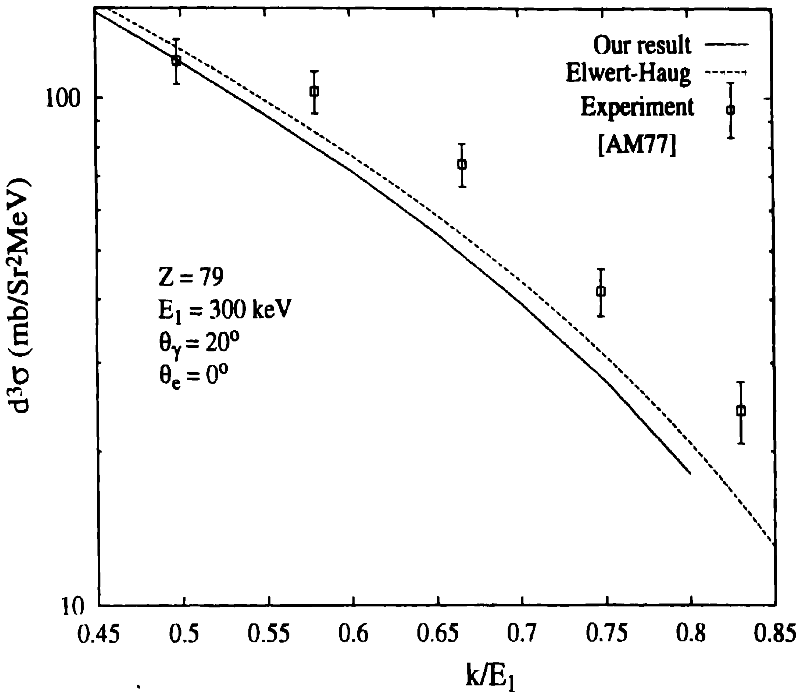

Fig. 1. Triply differential cross section for $Z = 79$, $E_1 = 300$ keV, $\theta\gamma = 20°$ and $\theta_e = 0°$, as a function of the fraction k/E_1 of incident energy radiated by the photon. Predictions of Shaffer et al., Elwert-Haug predictions including form factors, and experimental data are shown. The experimental data is from Fig. 4 of [24]. Figure taken from [23].

factor screening, and the experiments of Aehlig et al. [24] and Aehlig and Scheer [25]. Fig. 3 makes a similar comparison of theoretical predictions for the photon emission asymmetry from incident electrons spin polarized up or down normal to the scattering plane and the experiment of Mergl et al. [26]. It was concluded that at these energies the Elwert-Haug results, which should become good at high energies for all Z, were fair for $Z = 47$, poor (except perhaps for polarization) for $Z = 79$. Some agreement with experiment was found for $Z = 47$, with poor agreement (except perhaps for polarization) for $Z = 79$. (In the $Z = 79$ case, the experiments likewise did not support the Elwert-Haug results.) The conclusion was the hope that future, more accurate experiments, such as those now in progress, would hope to clarify the discrepancies between theory and experiment.

In subsequent work with the modified code, more systematic comparisons have been made of these partial-wave results (PW) with Elwert-Haug

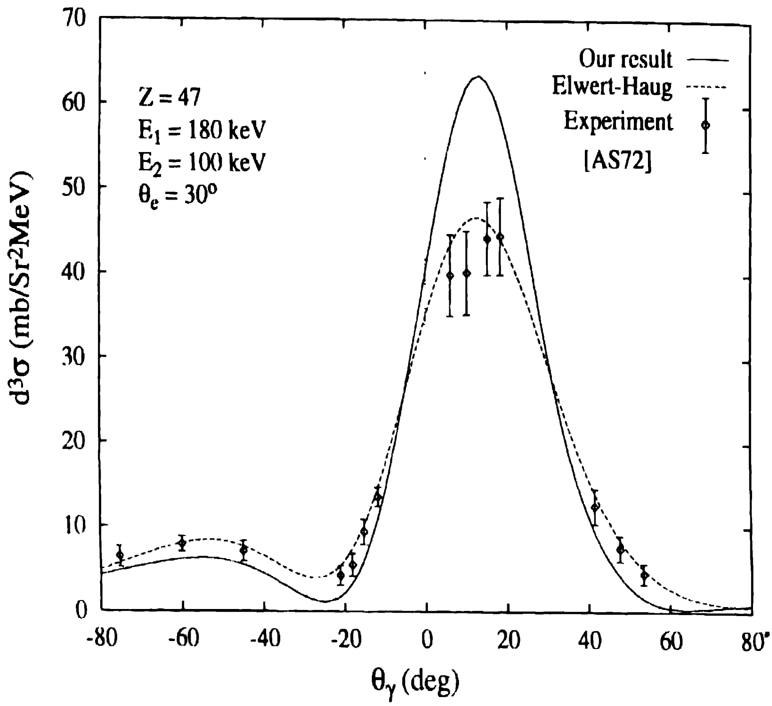

Fig. 2. Triply differential cross section for $Z = 47$, $E_1 = 180$ keV, $E_2 = 100$ keV and $\theta_e = 30°$, as a function of photon angle. Predictions of Shaffer et al., Elwert-Haug predictions including form factors, and experimental data are compared. The experimental data is from Fig. 2 of [25]. Figure taken from [23].

(EH) predictions. It was found that EH seldom overestimates the cross section by more than 10%, while generally it is smaller than PW, corresponding to Fink's observation [27] that it is smaller in $d^2\sigma$. When examining non-coplanar situations, the absolute difference between the two predictions was not significantly larger than in the coplanar case. For these energies, outgoing electron and photon directions are fairly well correlated and the near-forward peaking of $d^3\sigma$ is not yet very sharp, qualitative features already seen in Born approximation. For emission at larger angles, where the cross section is small, the relative difference between EH and PW is large.

7. What are we learning from studies of bremsstrahlung?

At high energies, many regimes of bremsstrahlung will be primarily determined in terms of external-field quantum electrodynamics (QED) in the

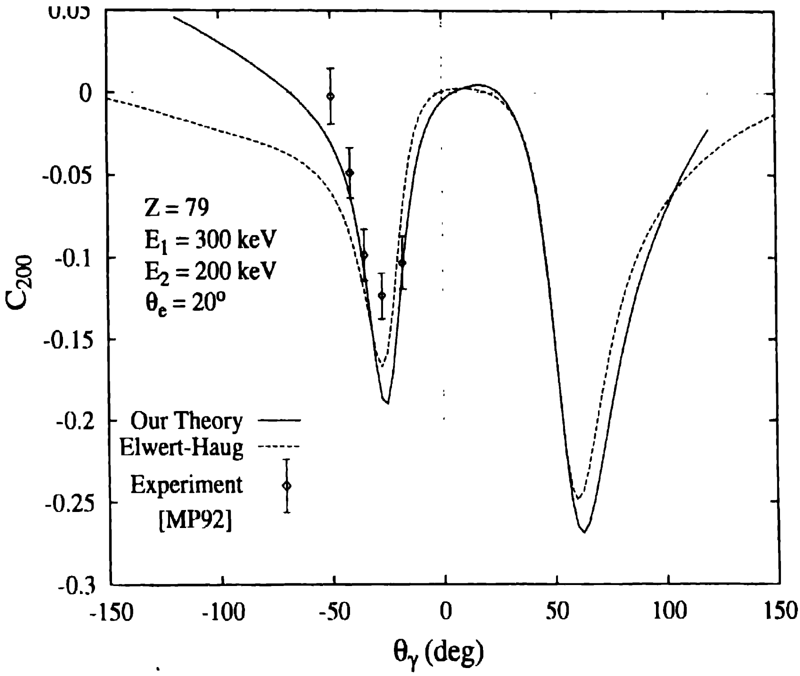

Fig. 3. Photon emission asymmetry C_{200} for $Z = 79$, $E_1 = 300$ keV, $E_2 = 200$ keV and $\theta_e = 20°$, as a function of photon angle. Predictions of Shaffer et al., Elwert-Haug predictions including form factors, and experimental data are compared. The experimental data is from Fig. 2 of [26]. Figure taken from [23].

nuclear point-Coulomb potential. The work on $d^3\sigma$ discussed in the previous section, may primarily be viewed as attempts to determine the adequacy of such an approach. Certainly there is no evidence, either in bremsstrahlung or in related processes such as pair production, photoeffect, Rayleigh and Compton scattering, etc., for any breakdown of the external-field QED approach. Likewise, there are no experimental reasons for anticipating any breakdown, or for believing these processes afford the most promising opportunities for observing deviations from the standard theory. On the other hand, for all these processes in the hard x-ray and soft γ-ray regimes, available data is very limited and of rather low accuracy; especially in totally differential situations which would provide more stringent tests. One cannot with any confidence say that theory and experiment are in agreement. Hence the tests for $d^3\sigma$ in bremsstrahlung which compare PW results with new experiments are welcome.

At low energies (x-ray and below), we can use bremsstrahlung to explore the transition from classical to quantum description, the role of many-body correlation effects, and the transition from a nonrelativistic to a relativistic description. A classical description is useful, at least for the spectrum, to quite high energy, as in many plasma applications. A nonrelativistic description of the spectrum persists into the soft γ-ray regime. These are both examples of the loss of sensitivity to model in integrated quantities that we have already mentioned. This still applies when the many-body correlations of polarizational bremsstrahlung are included, as when they are modeled classically. But in principle. more detailed experiments in the regime of polarizational bremsstrahlung should teach us about the response of atomic structures to these radiative processes. Once again, there is very little existing data, but new experiments are anticipated.

We may ask how the transition from a largely nonrelativistic dipole regime, sensitive to atomic screening of the nuclear point Coulomb-potential and sometimes to the many electron correlations of the atomic system, occurs. There is new information on some aspects of this question from studies of related processes [28]. In atomic photoeffect, one notes a transition from a largely dipole regime at low energies to a regime, involving increasing number of multipoles with increasing energy, but with matrix elements which become increasingly nuclear point Coulombic in character, except for the normalization of the initial bound state. To specify angular distributions and polarization correlations accurate to 1%, one only needs the deviation of the lowest multipole matrix elements from their nuclear point-Coulomb values: dipole differences suffice for states bound by less than 20 eV, dipole and quadrupole difference suffice for states bound by less than 5 keV, and for the most tightly bound states octupole differences also contribute. For total cross sections (i.e. again a more highly integrated quantity) much less atomic information enters: dipole differences suffice except for states bound by more than 5 keV, when quadrupole differences are also needed. Examples of these behaviours were shown in [28] for the total and differential cross section of the Uranium $3p_{1/2}$ subshell, as a function of ejected photoelectron energy, as screening is included in increasing numbers of multipoles. One may expect that this behavior, although established within independent particle approximation, will in most situations be more general. Thus one anticipates that, irregardless of energy, it should not normally be necessary to include many-body correlations beyond the lowest multipoles.

A related result has now been established in Rayleigh scattering, based on the realization that this process is well described in terms of modified form factors and angle-independent anomalous scattering factors. The form factor is determined by the screening of the nuclear point-Coulomb charge by the atomic electrons, and this simple dependence on atomic properties persists at all energies (unlike in photoeffect). But for the remainder, the angle-independent anomalous scattering factors, the story is the same as for photoeffect. This follows because the imaginary anomalous factor f'' is essentially the total photoeffect cross section, and the real anomalous factor f' is obtained from it through a dispersion relation. The situation on need for screening in higher multipoles does not change greatly even when the (weak) angular dependence of the anoamlous factors is considered.

From the foregoing one may anticipate the situation to be found in bremsstrahlung, since we know bremsstrahlung can be described in terms of a Born-approximation form-factor description (which becomes exact in the soft-photon regime of the sectrum for a potential with a long-range ionic-Coulomb tail) and a hard-photon regime (tip region of the spectrum) which is the analytic continuation of photoeffect. Thus, subtracting a Born-approximation description, only low multipoles should suffice to characterize the remaining screening effects in the cross section, becoming small with increasing energy. The approach reported by Avdonina for parameterizing the bremsstrahlung spectrum is related to this viewpoint.

A similar discussion can be given of the transition from nonrelativistic to relativistic descriptions. It has been known for some time [29] that total cross sections (but not differential cross sections) for photoeffect from s states is well given non-relativistically in dipole approximation even into the soft γ-ray regime. A systematic survey has been made more recently [30]. One can understand analytically how this cancellation of relativistic, retardation and higher-multipole effects comes about [31]; the poles of the matrix element in the energy plane are in the same position for the non-retarded dipole matrix element with nonrelativistic kinematics and for the retarded full-multipole matrix element with relativistic kinematics, but not in the mixed case. A similar situation applies for the spectrum (but not the angular distribution) in bremsstrahlung, and for the same reasons. This permits much simpler parameterization of the bremsstrahlung spectrum through the x-ray regime into the soft γ-ray regime.

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